HL 51: Nitrides: Preparation and Characterization

Time: Friday 9:30–12:15 Location: POT 112

HL 51.1 Fri 9:30 POT 112

High resistive buffer layers by Fermi-level engineering — •Armin Dadgar, Ralf Borgmann, and André Strittmatter — Otto-von-Guericke-Universität Magdeburg, FNW-IfP, Universitätsplatz 2, 39106 Magdeburg

We present a novel method to increase the resistivity of semiconductor buffer layers by aligning the Fermi level using a donor and an acceptor dopant of which one preferentially is a deep level placed in the lower (acceptor) or upper (donor) half of the energy band-gap. Potential doping sequences in GaN were simulated by nextnano software showing that the average Fermi-level position of alternately donor and acceptor doped layers can be shifted to the midgap position. This shift decreases the free carrier concentration and increases the resistivity as demonstrated for GaN:C / GaN:Si layer stacks. In structures grown by metalorganic vapor phase epitaxy, less charging and hysteresis effects are observed upon polarity changing between electrical contacts placed at surface and substrate. Also, the reduced total deep level concentration improves resistivity under electron and hole injection and the overall breakdown voltage by more than 20 %.

HL 51.2 Fri 9:45 POT 112

yolo-assisted object detection of dislocation-related pits on GaN surfaces using generative adversarial networks — •Mahdi Khalili Hezarjaribi[1,2], Uwe Rossow[1,2], Heiko Bremers[1,2], and Andreas Hangleiter[1,2] — [1]Institute of Applied Physics, Technische Universität Braunschweig, Germany — [2]Laboratory for Emerging Nanometrology, Technische Universität Braunschweig, Germany

In this paper, we present a model for detecting dislocation-related pits on GaN surfaces using SEM images, which strongly relies on the use of synthetic image generation. Pits mark dislocations in the layers and are widely used to assess crystalline quality; therefore, a considerable amount of images containing pits have to be evaluated. For this purpose, a Deep Learning (DL) algorithm is employed to achieve objective results, which are detecting the pits, and hence the dislocations, in SEM images. In order to train the algorithm to efficiently detect the objects, we need a host of SEM images containing pits in multiple sizes, numbers, formations, and noises. Due to the complexity of the microscopic structures and the lack of enough images, we incorporated a group of powerful algorithms called Generative Adversarial Networks to create artificial fake images just like real images and feed them, together with our real images, to our dataset to enrich the volume of the dataset. In the next stage, the YOLO algorithm (version 5) has been employed as the core deep learning algorithm for the object detection process using the above-mentioned dataset to train the network. A minimum average confidence of 86% for detecting real objects has been realized, corresponding to a high probability of detection.

HL 51.3 Fri 10:00 POT 112

Molecular beam epitaxy growth study and characterization of HoN thin films — •Anna Melendez-Sans[1], Vanda M. Pereira[1], Chun-Fu Chang[1], Chang-Yang Kuo[1,2,3], Chien-Te Chen[2], Liu Hao Tjeng[1], and Simone G. Altendorf[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]National Synchrotron Radiation Research Center, Hsinchu, Taiwan — [3]Department of Electrophysics, National Yang Ming Chiao Tung University, Hsinchu, Taiwan

Rare earth nitrides show potential for a wide range of applications due to their strong magnetic moment and semiconducting behavior. However, their synthesis and characterization has proven challenging since they rapidly oxidize when exposed to ambient conditions. Thanks to continuous developments in UHV-based thin film growth methods it is possible to grow high quality rare earth nitride films and, through the characterization of these, gain better insight into these compounds.

Whilst there have been many reports on GdN and SmN, not much is yet known about HoN. Now we present a systematic growth study on HoN thin films synthesized by molecular beam epitaxy (MBE), and using different substrates (MgO, $LaAlO_3$) and growth conditions (substrate temperatures and Nitrogen-gas pressure). These films were subsequently characterized using *in situ* techniques (Reflection high-energy electron diffraction, X-ray absorption and photoelectron spectroscopy) and *ex situ* techniques (X-ray diffraction, Superconducting quantum interference device) in order to evaluate their crystalline, electronic and magnetic structure.

HL 51.4 Fri 10:15 POT 112

Theoretical study on the (Al,Sc)N random alloy — •Jan M. Waack[1,2], Markus Kremer[1,2], Michael Czerner[1,2], and Christian Heiliger[1,2] — [1]Institut für theoretische Physik, Justus-Liebig-Universität Gießen, Germany — [2]Center for Materials Research (LaMa), Justus-Liebig-Universität Gießen, Germany

Aluminium scandium nitride ($Al_xSc_{1-x}N$, (Al,Sc)N or AlScN) is an random alloy. As such, the calculation of physical properties requires specific methods such as the coherent potential approximation (CPA)[1] and special quasi-random structures (SQS)[2]. We compare the CPA in the framework of the atomic sphere approximation (ASA) Korringa-Kohn-Rostoker (KKR) density functional theory (DFT) with the SQS using the plane-wave pseudopotential DFT to calculate the lattice parameters and electronic band structures of the face-centered cubic phase of $Al_xSc_{1-x}N$ (with $0 \leq x \leq 1$).

Using the low computational cost LDA-1/2 quasiparticle method [3] to calculate the electronic band structures within SQS and CPA, we present the first implementation of LDA-1/2 within the KKR DFT. We find that both the lattice parameter and the indirect band gap deviate from Vegard's law.

[1] C. Franz, M. Czerner, and C. Heiliger, Phys. Rev. B 88, 94421 (2013). https://doi.org/10.1103/PhysRevB.88.094421

[2] A. Zunger, S.-H. Wei, L. G. Ferreira, and J. E. Bernard, Phys. Rev. Lett. 65, 353 (1990). https://doi.org/10.1103/PhysRevLett.65.353

[3] L. G. Ferreira, M. Marques, and L. K. Teles, Phys. Rev. B 78, 125116 (2008). https://doi.org/10.1103/PhysRevB.78.125116

HL 51.5 Fri 10:30 POT 112

Thermal Transport in c-plane GaN Membranes Studied by Raman Thermometry — •Wilken Seemann[1], Joachim Ciers[2], Isabell Hüllen[1], Mahmoud Elhajhasan[1], Jean-François Carlin[3], Nicolas Grandjean[3], Åsa Haglund[2], and Gordon Callsen[1] — [1]Institute of Solid State Physics, University of Bremen, Germany — [2]Department of Microtechnology and Nanoscience, Chalmers University of Technology, Gothenburg, Sweden — [3]Institute of Physics, École Polytechnique Fédérale de Lausanne (EPFL), Switzerland

Heating during operation often limits the lifetime or stability of semiconductor devices, like laser structures, e.g., via defect formation or by affecting the refractive index. Understanding how thermal energy is dissipated from the active region of such structures is therefore an important step towards device optimization.

We analyze the in-plane thermal transport in GaN-based membranes. The temperature is probed by the shift and width of Raman modes under heating with a UV laser. This allows for a non-contact characterization without the need for additional processing steps.

By varying the membrane underetching process, we can tune the membrane bottom facet roughness and porosity to study their impact on thermal conductivity κ, due to phonon boundary scattering. A reduction of κ is a sign of phonon frequency filtering, which is a first step towards engineering the phonon dispersion relation in GaN membranes. Controlling this effect, e.g., via the position and sizes of pores, might enable thermal concepts to locally reduce temperature rises.

15 min. break

HL 51.6 Fri 11:00 POT 112

SmN thin films: MBE-growth and spectroscopy studies — •Vanda M. Pereira[1], Anna Melendez-Sans[1], Chun-Fu Chang[1], Chang-Yang Kuo[1,2,3], Chien-Te Chen[2], Liu Hao Tjeng[1], and Simone G. Altendorf[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]National Synchrotron Radiation Research Center, Hsinchu, Taiwan — [3]Department of Electrophysics, National Yang Ming Chiao Tung University, Hsinchu, Taiwan

Although the rare earth nitrides have been in the scientific scene for many decades, their poor stoichiometry and reactivity in ambient conditions have severely conditioned their progress. It has been only rather recently that studies on thin films have started to unveil some of their unique characteristics and solve decades-old controversies, but there

are still significant gaps left to explore.

Recent studies on the ferromagnetic semiconductor SmN suggest that the $4f$ bands are involved in electron transport and are crucial to the observed superconductivity in nitrogen-vacancy doped samples. Nevertheless, more concrete experimental evidence is needed.

Here we present a systematic study of SmN thin films grown by molecular beam epitaxy, exploring their crystalline quality and composition as the growth parameters (substrate temperature and nitrogen pressure) are varied. The films were characterized *in situ* making use of photoemission and x-ray absorption spectroscopies, thereby allowing to reliably gain more insight into the electronic structure of this material.

HL 51.7 Fri 11:15 POT 112

Growth of ScN and AlScN by reactive sputter epitaxy — •Florian Hörich, Christopher Lüttich, Ralf Borgmann, Jürgen Bläsing, André Strittmatter, and Armin Dadgar — Otto-von-Guericke University

Spontaneous polarization fields induced by a strained AlGaN/GaN layer structure lead to high-density two-dimensional electron gases which are key to current high-power and high-frequency transistor devices. Recent theoretical and experimental data demonstrated an even higher two-dimensional electron density when AlScN is used [1]. Up to now, growth of Sc-containing materials by conventional MOVPE is hampered by the lack of a suitable Sc precursor. Reactive sputter epitaxy using metallic Al and Sc targets together with ammonia or molecular nitrogen has the potential to fabricate high quality layers at low cost. We will discuss principle growth parameters such as temperature and nucleation conditions for ScN and AlScN on bare Si(111) substrates and on MOVPE grown GaN templates. A large impact of growth temperature is observed on crystal structure and surface morphology. Single-phase crystalline material is obtained at temperatures $>$ 800 °C. We find different optimum nucleation conditions for both kind of substrate surfaces. Growth on bare Si(111) surfaces with an initial metallic Sc thickness equivalent to $<$1 nm drastically improves crystallinity. For the GaN(0001) template surface, such sequence has no impact. Additionally, sputtering of AlScN and ScN with ammonia results in better structural quality than with nitrogen.

[1] I. Streicher, et. al. Phys. Status Solidi RRL 2200387

HL 51.8 Fri 11:30 POT 112

On the variation of PL intensity in GaInN/GaN quantum wells with different cladding thicknesses — •Nico Wagner[1], Shawutijiang Sidikejiang[1,2], Philipp Henning[1,2], Rodrigo de Vasconcellos Lourenço[1,2], Heiko Bremers[1], Uwe Rossow[1,2], and Andreas Hangleiter[1,2] — [1]Institute of Applied Physics, Technische Universität Braunschweig, Germany — [2]Laboratory for Emerging Nanometrology, Braunschweig, Germany

The absolute internal quantum efficiency (IQE) of GaInN/GaN quantum wells (QW) at low temperature can be determined using time-resolved photoluminescence (PL) measurements. If the IQE is 100 %, the PL intensity under steady state conditions is expected to be the same for all samples. We can verify that for some samples, but others show different intensities. It turns out that the difference varies for different cladding thicknesses, i.e. the layer between the QW and air. In this work, we present a model calculating the allowed modes inside the sample assuming that all the light is emitted into them if we have 100 % IQE. Due the small critical angle, it is important to determine the small ratio of intensity, which is coupled out and detected. The result yields an oscillating behavior as a function of the cladding thickness and shows a good agreement with the measured samples. It is important to note that this is a consequence of the Purcell effect, i.e. that spontaneous emission depends on the optical environment.

HL 51.9 Fri 11:45 POT 112

Optical properties of ScN films grown by HVPE and sputter epitaxy — •Jona Grümbel[1], Yuichi Oshima[2], Christopher Lüttich[1], Armin Dadgar[1], Martin Feneberg[1], and Rüdiger Goldhahn[1] — [1]Institut für Physik, Otto-von-Guericke-Universität, Universitätsplatz 2, 39106 Magdeburg — [2]Environment and Energy Materials Research Division, National Institute for Materials Science, 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan

We investigate the optical properties of rocksalt structured ScN films using spectrocopic ellipsometry and Raman spectroscopy. Two different sets of samples were used for our measurements: (I) ca. 300nm thick ScN grown by sputter epitaxy and (II) 0.4μm up to 40μm thick ScN grown by HVPE. The HVPE grown ScN exhibits a very good crystalline structure, so the carrier concentration varies around 10^{18}cm^{-3} - 10^{19}cm^{-3}, while for ScN grown by sputter epitaxy the carrier concentrations can reach 10^{22}cm^{-3} or more. Therefrom we obtain detailed information about their impact on optical properties, such as optical transitions, optical phonon modes or luminescence. Using spectroscopic ellipsometry we arrive at the dielectric function of ScN from 0.04eV to 6.5eV. Detailed analysis yields the main transitions regarding to direct bandgaps at X- and Γ-point as it was already shown in earlier theoretical works. Surprisingly, we observe characteristic peaks in a Raman scattering measurement, although first order Raman scattering is forbidden in rocksalt structured crystals. Detailed discussion and a possible interpretation will be presented as well as ScN materials parameters calculated from our measurements.

HL 51.10 Fri 12:00 POT 112

Temperature dependent spectroscopic ellipsometry on cubic GaN — •Jonas Rose[1], Elias Baron[1], Rüdiger Goldhahn[1], Michael Deppe[2], Donat J. As[2], and Martin Feneberg[1] — [1]Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Germany — [2]Department Physik, Universität Paderborn, Germany

Cubic Galliumnitride (c-GaN) is a promising material for designing and fabricating efficient optoelectronic devices, such as green LEDs, and can potentially replace hexagonal GaN for certain applications due to its lack of internal polarization fields. Therefore, the knowlegde and control of the optical properties is essential. Recently, several breakthroughs regarding crystal quality of c-GaN have been achieved by utilizing 3C-SiC as a substrate material. We present our investigation of thin film c-GaN deposited by plasma-assisted molecular beam epitaxy on 3C-SiC/Si substrates in (001) orientation. Temperature dependent spectroscopic ellipsometry between 80 and 300 K yields the optical properties (dielectric function, DF) in this temperature range. Hereby, the influence of the excitonic contribution to the DF is of special interest. Using Elliott's model, we describe the lineshape of the DF around the absorption onset. The obtained transition energies follow Pässler's temperature dependent model. Degenerately doped samples up to 10^{20} cm^{-3} are investatigated as well. A free-carrier dependent behaviour of the absorption onset is observed and explained for different temperatures.